Nature of semiclassical spectrum in terms of classical trajectories.

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半古典量子化のメカニズムを詳細に検討し、半古典スペクトルの構成には、量子化される軌道だけでなく、量子化されるスペクトルの倍音等の間違ったスペクトルを消す軌道が重要な役割を果たすことを明らかにした。こうした研究に基づき、効率的に半古典スペクトルを計算する方法を提案し、２次元カオス系に適応した。さらに、この方法の利点を生かして固有状態に対応する古典軌道を抜き出し、その性質について議論した。

〔Abstracts〕

The mechanism of semiclassical quantization is examined in detail. We found an important role of destructive interference in building quantum spectrum. Based on this analysis, we propose an efficient method to calculate the semiclassical spectrum. This method is particularly promising in multidimensional chaotic systems and also very useful to identify which trajectories dominate a quantum spectrum. We numerically examine this method by applying to a two-dimensional chaotic system and show an illustrative example of identifying such a dominant trajectory that corresponds to an eigenstate.

〔AFC-II〕

In this paper, we use an amplitude-free quasi-correlation function type-II (AFC-II) for the calculation of semiclassical correlation function. (Note that our proposed method is general and can apply to any semiclassical theory.) In AFC-II scheme, Fourier Transformation of the following amplitude-free quasi- correlation function obtains semiclassical spectrum [1],

$$C(t)=\langle\Psi(q,0)|\Psi(q,t)\rangle=\sum_{q_0}\left(\frac{\alpha}{\pi}\right)^{\frac{1}{2}}\exp\left(-\frac{\alpha(q-q_m)^2}{2}\right)\exp\left(\frac{i}{\hbar}S(q,q_0,t)-\frac{i\pi}{2}M\right)\exp\left(-\frac{\alpha(q_0-q_m)^2}{2}\right)$$

where q_m is a central position of an initial wave packet and α is its width. Only classical trajectories, which start from q_0 with zero momentum (called the turn-back orbits), are sampled (For the details and reasons why pre-factor does not appear in the above formula, see Ref. 1). One of the advantages of AFC-II is that the correlation function is amplitude-free. It is important for the application to chaotic systems, since the pre-factor in a chaotic system becomes large and tend to infinity. The other advantage is that the sampling of trajectories is easy. Different from the periodic orbit theory, we do not need to search periodic orbits, which is tough task.

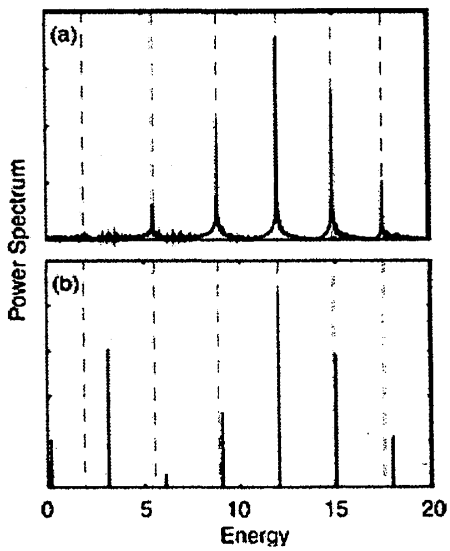

Fig.1 Semiclassical spectrums

〔Mechanism of semiclassical quantization〕

First, let us start from a one-dimensional simple case. Here we use Morse potential $V(x)=30(1-\exp(-0.5x))^2$ as an example. We choose mass and $\hbar$ equal one.

Spectrum obtained by AFC-II with 1000 sampling paths is shown in Fig. 1(a). We also show analytic obtained quantum eigenvalues as dotted lines. Semiclassical spectrums are in good agreement with the quantum eigenvalues.

Next, we analyze how to build semiclassical spectrum as follows [2, 3]. Power spectrum is obtained by Fourier transformation of AFC-II. Here we change the order of sum and time integral such as

$$\begin{aligned} P(E) &= \int dt \sum_{q_0} \left|F(q_t)F(q_0)\right| \exp\left(\frac{i}{\hbar}S(q,q_0,t) - \frac{i\pi}{2}M\right)\exp\left(\frac{i}{\hbar}Et\right) \\ &= \sum_{q_0} \int dt \left|F(q_t)F(q_0)\right| \exp\left(\frac{i}{\hbar}S(q,q_0,t) - \frac{i\pi}{2}M\right)\exp\left(\frac{i}{\hbar}Et\right) \\ &= \sum_{q_0} P_{q_0}\left(E_{cl}(q_0);E\right) \end{aligned}$$

Single spectrum $P_{q_0}\left(E_{cl}(q_0);E\right)$ is calculated by only one single trajectory and the sum of the single spectrum is equivalent to the total power spectrum. We analyze each single spectrum and examine which classical trajectory and how each trajectory contributes to spectrum.

--Constructive interferences--

Figure 1(b) shows an example of single spectrums which gives the largest contribution to the eigenstate n=4. The energy of the most contributing trajectory is almost equivalent to the quantized energy, 12.02. The most important fact is quantized state can be obtained mainly by one classical trajectory. However, only from one trajectory, we also obtain incorrect spectrums (harmonic overtones of the correct spectrum) as seen in Fig.1 (b).

The stationary phase condition of the Fourier transformation of the semiclassical correlation function is such as

$$\frac{\partial}{\partial t}\left(S(q,q_0,t)+Et\right) = -E_{cl}+\varepsilon = 0$$

This formula shows that the trajectory with energy E_{cl} mainly contributes to the spectrum at $\varepsilon = E_{cl}$. Therefore the quantized spectrum can be built by a single trajectory with quantized energy. We call this contribution *constructive interference* (CI). CI is interferences within one trajectory and builds a correct spectrum.

--Deconstructive interferences--

Next we examine how trajectories contribute to each spectrum. Single spectrums at three target energies E_{target}, $P_{q_0}\left(E_{cl}(q_0);E_{\text{target}}\right)$, are plotted as a function of energy of sampling trajectories E_{cl} in Figs. 2 (a)-(c). First we pick up E_{target}=5.528, which corresponds to n=1 in a panel (a). In this case, trajectory with quantized energy contributes to the spectrum most. We next choose E_{target}=5.553, just deferent from quantized energy. The contribution from a trajectory with E=5.553 is small in Fig.2 (b). Because summation of all the contribution becomes spectrum at E=5.553, the sum of

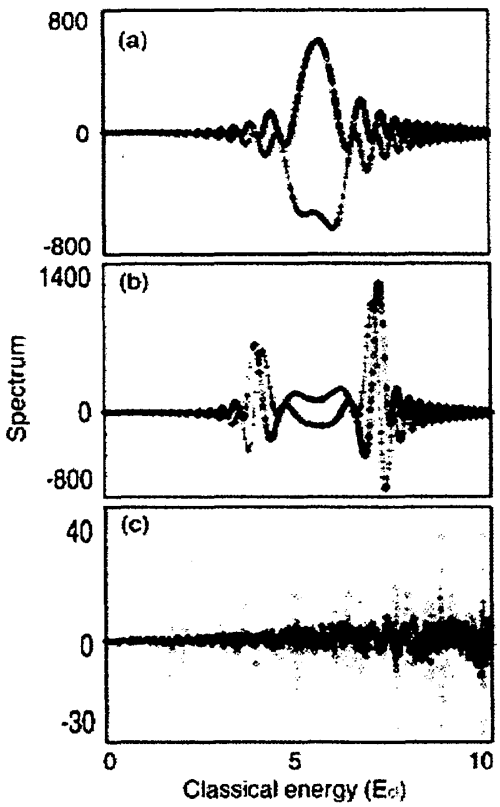

Fig.2 Single spectrum Ecl for selected E.

vibrational parts must become zero. To converge this oscillatory integral, we need a huge number of trajectories. Last example is E_{target}=7.210 in Fig.2 (c). It is just between quantized energies and we cannot find any structure. In this case, the summation of all the contribution to this energy should be zero, too.

As we see above, to erase incorrect spectrums, many trajectories with non-quantized energies are necessary. We call this process *deconstructive interference* (DI). DI is interference between trajectories and erases the incorrect spectrums. To do so, we need a huge number of trajectories and this is why we need a huge number of trajectories to calculate semiclassical spectrum.

〔An efficient filtering technique to take account of CI and DI〕

From the above investigations, we understand there are two types of interferences (CI and DI) and both play an important role in building semiclassical spectrum. One of the numerical difficulties in semiclassical theory is numerical evaluation of oscillatory integrals, which represent DI. To perform efficient estimation of the oscillatory integrals, we introduce window function in the power spectrum such as

$$\tilde{P}_{[W]}(E)=\int dt\sum_{q_0}\Delta_W\left(E-E_{cl}(q_0)\right)\left|F(q_t)F(q_0)\right|\exp\left(\frac{i}{\hbar}S(q,q_0,t)-\frac{i\pi}{2}M\right)\exp\left(\frac{i}{\hbar}Et\right)$$

where $\Delta_W\left(E-E_{cl}(q_0)\right)$ is a window function that filter out the components located out of energy range [2, 3].

In the case of the quantized trajectories, if we use window function, only CI alive and incorrect spectrums (harmonic overtones) disappear. On the other hand, in the case of non-quantized trajectories, we cannot consider DI with narrow window functions. However, it is not necessary because we neglect incorrect spectrums (harmonic overtones) constructed by a quantized single spectrum. Although we must test several types of window functions, we can expect that we need a small number of trajectories to evaluate semiclassical spectrums.

〔Numerical examples〕

Here we test the above-proposed method in the modified Hénon-Heiles system [3]. Hamiltonian is written such as

$$H=\frac{p_x^2}{2m_x}+\frac{p_y^2}{2m_y}+\frac{x^2+y^2}{2}+x^2\left(0.6y^2+y\right)+\frac{y^3}{3}\left(0.2y-1\right)+0.1x$$

with $m_x=1.0087$, $m_y=1.0$, and $\hbar=0.005$. Here we examine highly excited states, which locate between 0.13 and 0.16. In this energy range, almost all the phase space is filled with chaotic sea.

First we choose the width of window as small as the grid spacing of numerical Fourier transformation. In this case, we simply note W=1. Semiclassical spectrum with W=1, W=4, W=10, and W=∞ are examined and shown in Fig.3 (a), (b), (c), and (d), respectively. W=∞

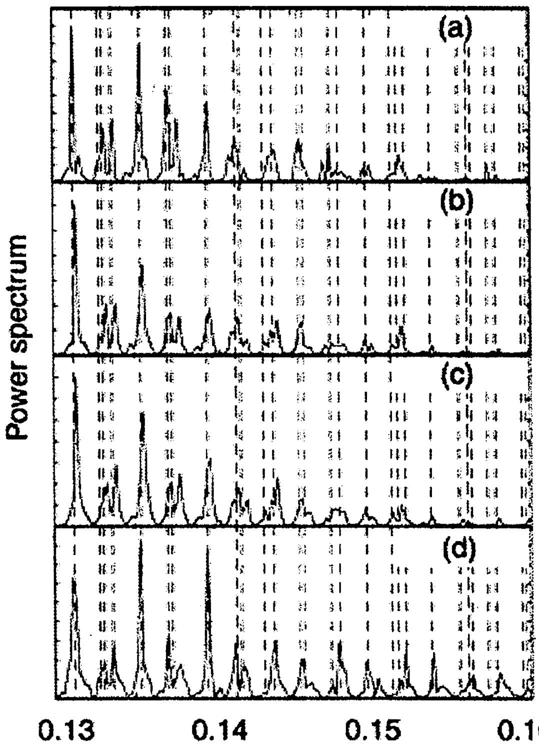

Fig.3 semiclassical spectrum with windows is equivalent to the original AFC-II spectrum. Quantum eigenvalues are shown as dotted lines. As the width of window function becomes wider, the shape of spectrum becomes similar one with W=∞. In every case, the agreement of semiclassical spectrum and quantum ones is excellent. Since we use the smallest number of trajectories in W=1, we recommend W=1 to estimate semiclassical spectrum in this system.

Next, we examine the most contributing trajectory on spectrum [3]. Here we use delta function as a window function, so that we can extract the trajectory, which corresponds to each spectrum. In Fig.4, we show the most contributing trajectory to the spectrum at E=0.13592 in a panel (a) which should be compared with the absolute square of the corresponding eigenfunction displayed in a panel (b). Since the nodal pattern of eigenfunction in Fig.4 (b) is irregular especially at a central part of eigenfunction, it seems to be difficult to quantize by the ordinary EBK condition. The spatial distributions of the trajectory in Fig.4 (a) and eigenfunction in Fig.4 (b) are similar to each other. One can find an apophysis around the center of eigenfunction in Fig.4 (b). It corresponds to thin bundle of trajectory that appears upper part of the thick bundle of trajectory located at the center of Fig.4 (a).

In this way, one can extract a few trajectories that are responsible for CI to build an eigenfunction. This example shows that we can examine nature of eigenfunction in terms of classical trajectories. For example, this technique seems to be very useful for the investigation of scar in chaotic systems.

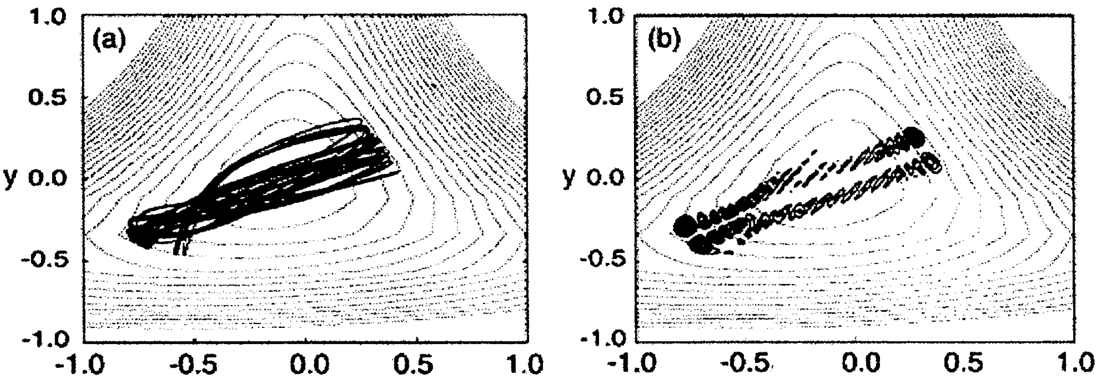

Fig.4 The most contributing trajectory and corresponding eigenfunction

〔Concluding remarks〕

In this paper, we first analyze how to build semiclassical spectrum. We found that there are two types of contribution, one is constructive and the other is deconstructive interference. Quantized trajectories not only construct correct spectrums but also build incorrect spectrum such as harmonic overtones. Non-quantized trajectories deconstruct incorrect spectrums. Both types of trajectories are important for building semiclassical spectrum.

Based on the above analysis, we introduce filtering technique for the calculation of semiclassical spectrum. We apply this method to a two-dimensional chaotic system and nature of spectrum has been examined in terms of trajectories. This example shows that our proposed method may give new insight into the quantum-classical correspondence.

〔References〕

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